hydrogen storage in nanoporous materials for aerospace applications

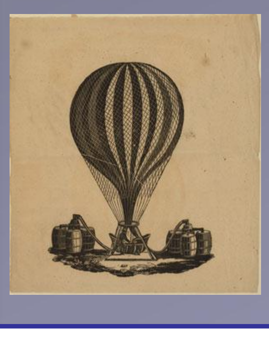
Jessica E. Sharpe,[a,b] Andrew D. Burrows,[c] Agata Godula-Jopek,[d] Timothy J. Mays[b]

[a] Doctoral Training Centre, Centre for Sustainable Chemical Technologies, [b] Department of Chemical Engineering, [c] Department of Chemistry, University of Bath, BA2 7AY, UK. [d] EADS Innovation Works, 81 663 Munich, Germany.

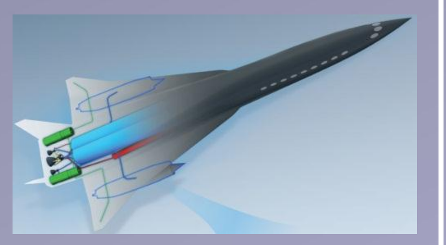
E-mail: J.Sharpe@bath.ac.uk: URL: http://people.bath.ac.uk/cestjm/, http://www.bath.ac.uk/csct

1. Introduction to hydrogen in aerospace applications

Timeline of hydrogen (H_2) within aerospace:

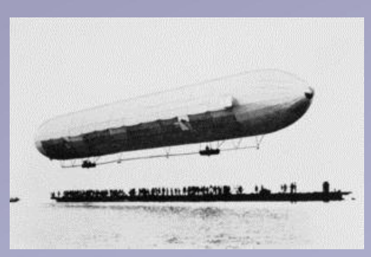
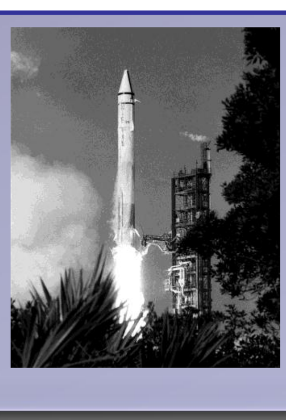






1783 – First hydrogen balloon flight	1954– Hydrogen peroxide Sikorsky Helicopter	1966 – Hydrogen batteries in satellite (NTS-2)	1988– First hydrogen aircraft prototype (Tupolev Tu-155)	C21st – EADS 'ZEHST' – High speed transport concept study

1900 – First airship flown purely on hydrogen (Zeppelin LZ1)	1966 – Hydrogen used as a rocket fuel (Atlas-centaur launch vehicles)	1969 – Hydrogen cryocooler on Mariner 6	2011 - Lange Aviation/DLR Antares H3 – hydrogen fuel cells (piloted and unmanned), 6000 km, >50 hrs[1]

Why we need H_2 in aerospace:

- Climate change
- Depletion of fossil fuels
- Lots of emissions in upper atmosphere

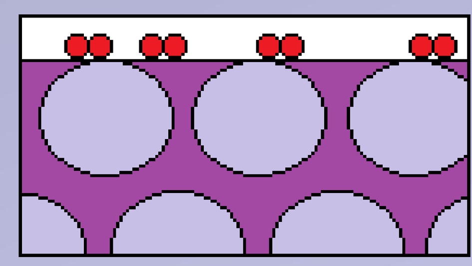
Therefore

Problem:

- Storage of H_2
  - Very low energy per unit volume => density must be increased.

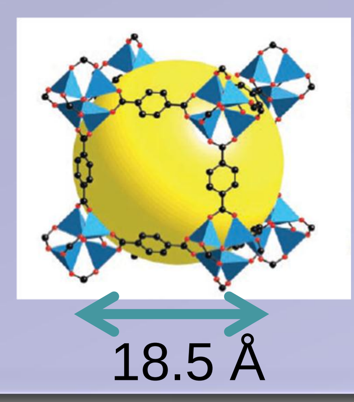
Solution:

➢ **Physisorption onto a porous material**



Desired properties of materials:

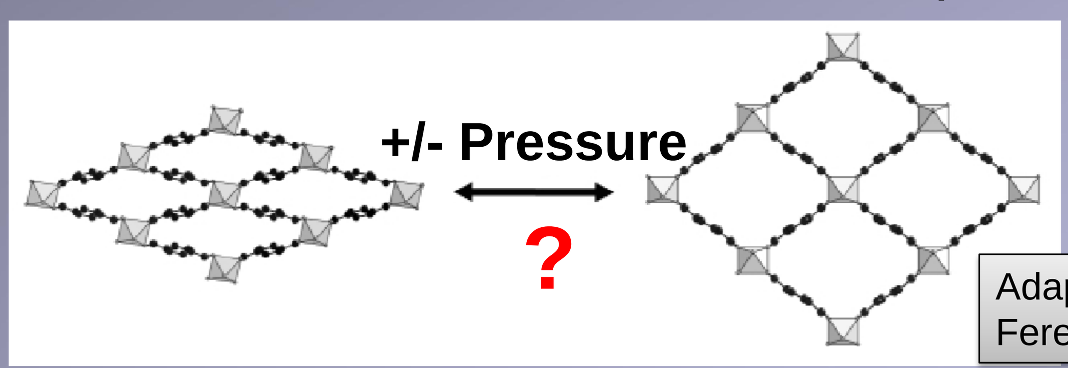
- *Light*
- *Robust*
- *Low cost*
- *High surface area*
- *Large pore volume*
- *Good cycle life*



E.g.
-Metal-organic frameworks (MOFs)
-Activated carbons
-Polymers of intrinsic microporosity (PIMs)

2. Research focus 1: Flexible MOFs

All conventional models assume a fixed pore volume, but:



Adapted from Ferey *et. al.*[1]

n_e – excess uptake
V_a – pore volume
ρ_a^{max} – maximum density
V_a^0 – initial pore volume
P - pressure
Z – compressibility factor
R – gas constant
T – temperature
α, β - parameters
ρ - density
($_b$ - bulk, $_a$ - pores, $_s$ - skeletal)
f – fill factor
ϑ_a – pore volume

We have created a mathematical model for this to fit to experimental isotherms:

$$n_e = V_a(\rho_a^{max}(isotherm\ equation) - \frac{P}{ZRT})$$

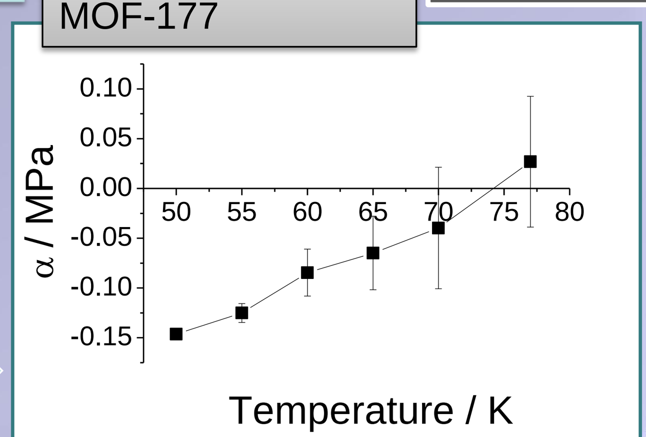
$$V_a = V_a^0(1 + \alpha P + \beta P^2 + \cdots)$$

Initial assumption:

$$V_a = V_a^0(1 + \alpha P)$$

Clear positive trend observed

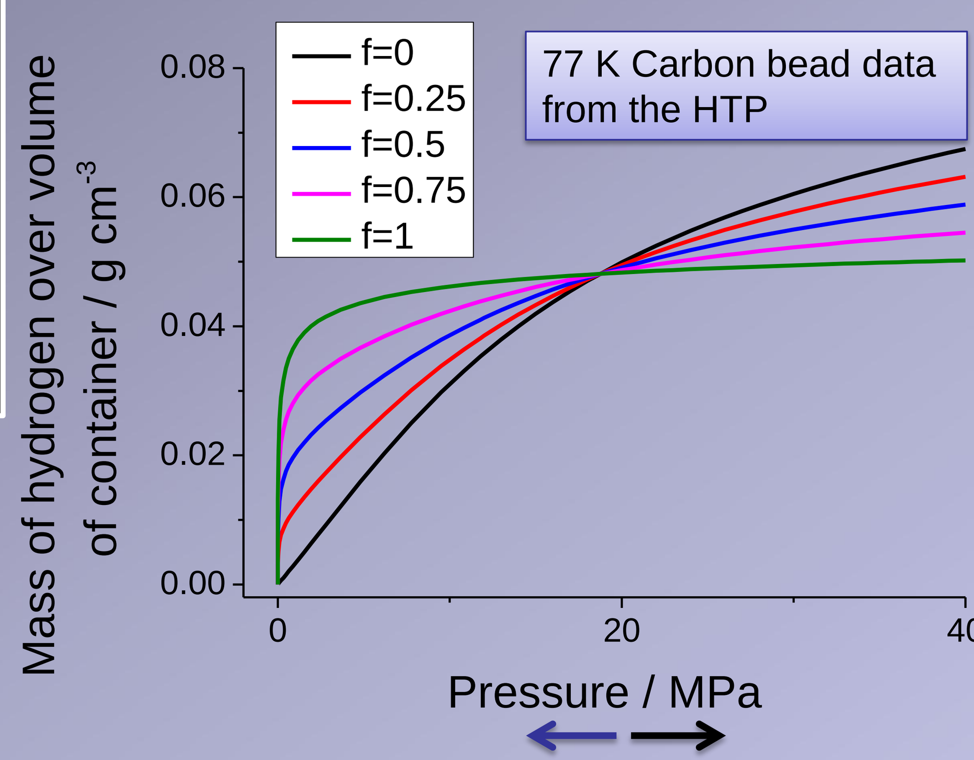
Alpha dependence on temperature for MOF-177



3. Research focus 2: Design curves

Direct comparison of adsorption vs. compression.

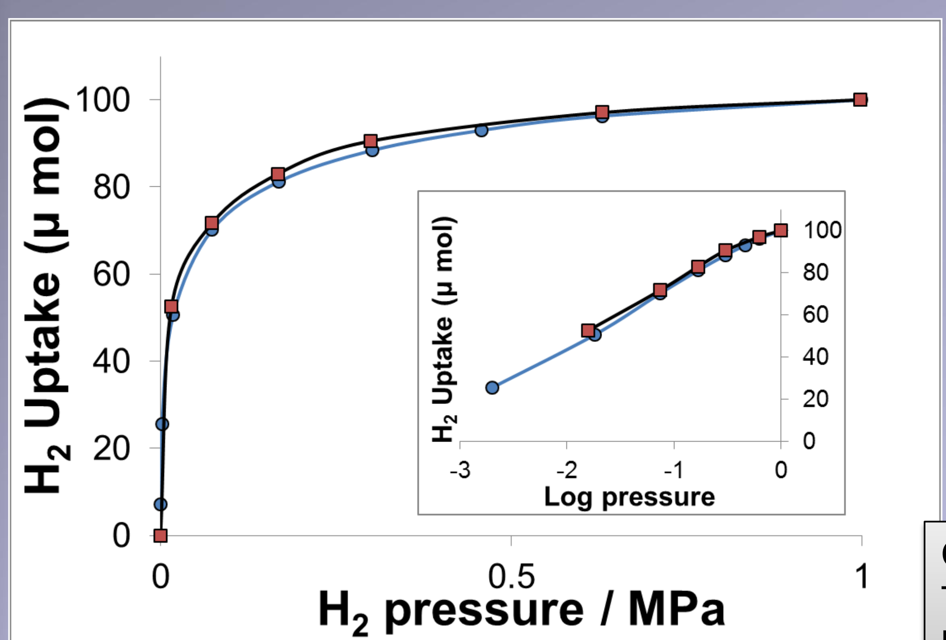
$$\frac{m_H}{V_c} = (1-f)\rho_b + f\rho_a\left(\frac{\vartheta_a\rho_s}{\vartheta_a\rho_s + 1}\right)$$



- Can get out a critical pressure, under which adsorption stores more hydrogen than compression in the same volume.
- Need to do mass of hydrogen over mass of the system to account for additional weight of adsorbent.

4. Research focus 3: Neutron scattering

Using inelastic neutron scattering to characterise H_2 adsorption in a novel way, and verify our experimental data.



Calculated integrated intensity of the TOSCA INS elastic peak (red sq.) and the hydrogen isotherm obtained in a volumetric gas analyser (blue circles).

- As seen, there is a very good match between the two sets of data.
- We are now going to try with different materials and at higher pressures.

5. Future work

- Continuation of stated work.
- Multipurpose Simulation Code (MUSIC) – to model H_2 uptake at conditions inaccessible in the lab.
- Looking at whole containment systems for H_2 adsorption

6. Outcomes for EADS

- To bring key data on potential materials for H_2 adsorption.
- Growing importance for **Astrium**, **Cassidian** and **Airbus**.

References:
1. Ferey, G.; Latroche, M.; Serre, C.; Millange, F.; Loiseau, T.; Percheron-Guegan, A., Hydrogen adsorption in the nanoporous metal-benzenedicarboxylate M(OH)(O_2C-C_6H_4-CO_2) (M = Al^{3+}, Cr^{3+}), MIL-53. *Chemical Communications* **2003**, (24).